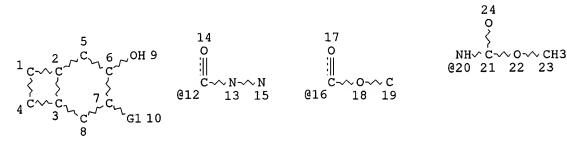
10/656617

(FILE 'REGISTRY' ENTERED AT 14:32:45 ON 09 MAR 2005)

L16

STR



VAR G1=N/12/16/20 NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 23

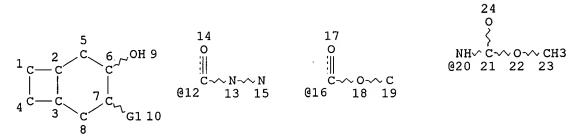
STEREO ATTRIBUTES: NONE

L18

19 SEA FILE=REGISTRY SSS FUL L16

L21

STR



VAR G1=N/12/16/20 NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RSPEC I

NUMBER OF NODES IS 23

STEREO ATTRIBUTES: NONE

L22 5 SEA FILE=REGISTRY SUB=L18 SSS FUL L21

100.0% PROCESSED 8 ITERATIONS

5 ANSWERS

SEARCH TIME: 00.00.01

FILE 'CAPLUS' ENTERED AT 14:36:09 ON 09 MAR 2005

L23 3 S L22

L23 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1973:525681 CAPLUS

10/656617

DOCUMENT NUMBER:

79:125681

TITLE:

Conformation and reactivity of [4.n.0]bicyclo systems

with trans ring junctions. XIX. Synthesis, conformation, and configuration of 4-Methyl- and 4-halobicyclo[4.2.0]octan-3-ols and -3-ones. Epimerization equilibriums for α -substituted

bicyclo[4.2.0]octanones

AUTHOR(S):

Casadevall, E.; Largeau, C.; Moreau, P.; Bouisset, M.

CORPORATE SOURCE:

Ec. Natl. Super. Chim., Paris, Fr. Tetrahedron (1973), 29(13), 1865-75

CODEN: TETRAB; ISSN: 0040-4020

DOCUMENT TYPE:

Journal

LANGUAGE:

SOURCE:

French

The conformations and configurations of trans-fused 4-bromo-, 4-chloro-, 4-fluoro-, and 4-methylbicyclo[4.2.0]octan-3-ols and -3-ones, prepared from 3,4-epoxybicyclo[4.2.0]octane and HBr, HCl, Me2CHNH3F, and MeLi, resp., were determined by ir, PMR, and uv spectroscopy. The epimerization equils. were determined for the bromo and chloro ketones in AcOH, CCl4, and dioxane, for the fluoro ketones in CCl4 and dioxane, and for the Me ketones in

41441-83-2P 49785-38-8P 49785-45-7P ΙT

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of)

RN41441-83-2 CAPLUS

Bicyclo[4.2.0]octan-3-ol, 4-(dimethylamino)-, CN

 $(1\alpha, 3\alpha, 4\beta, 6\beta)$ – (9CI) (CA INDEX NAME)

Relative stereochemistry.

49785-38-8 CAPLUS RN

Butanedioic acid, 2,3-bis(benzoyloxy)-, $[R-(R^*,R^*)]$ -, compd. with $(1\alpha, 3\alpha, 4\beta, 6\beta) - 4 - (dimethylamino) bicyclo[4.2.0] octan-3$ ol (9CI) (CA INDEX NAME)

CM 1

41441-83-2 CRN C10 H19 N O CMF

Relative stereochemistry.

571-272-2528 Searcher : Shears

CM 2

CRN 2743-38-6 CMF C18 H14 O8

Absolute stereochemistry.

RN 49785-45-7 CAPLUS

CN Bicyclo[4.2.0]octan-3-ol, 4-(dimethylamino)-, $(1\alpha, 3\alpha, 4\beta, 6\beta)$ -, compd. with 2,4,6-trinitrophenol (9CI) (CA INDEX NAME)

CM 1

CRN 41441-83-2 CMF C10 H19 N O

Relative stereochemistry.

CM 2

CRN 88-89-1 CMF C6 H3 N3 O7

L23 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:

1973:158766 CAPLUS

DOCUMENT NUMBER:

78:158766

TITLE:

Conformation and reactivity of trans-fused

bicyclo[4.n.0] compounds. XVIII. Spectroscopic study

of the conformational equilibrium of trans-fused

4a-dimethylaminobicyclo[4.3.0]nonan-3a-ols and of 4a-dimethylaminobicyclo[4.2.0]octan-3a-ols

AUTHOR(S):

Casadevall, Andre; Casadevall, Eliette; Moner,

Maryvonne

CORPORATE SOURCE:

Ec. Natl. Super. Chim., Paris, Fr.

SOURCE:

Bulletin de la Societe Chimique de France (1973),

(2) (Pt. 2), 657-62

CODEN: BSCFAS; ISSN: 0037-8968

DOCUMENT TYPE:

Journal

LANGUAGE:

French

AB The ir spectra of the trans-diaxial-dimethylaminobicyclo[4.3.0]nonanols and of the trans-diaxial-dimethylamino-trans-bicyclo[4.2.0]octanols were observed in the OH stretch region and the free and bound OH bands assigned. The temperature dependence of the OH bands was interpreted in terms of an equilibrium

between a chair conformation, in which H-bonding was intermol., and a flexible conformation in which H-bonding was intramol.; the equilibrium thermodn. parameters were calculated The disagreement between the NMR and

ir

temperature dependencies of the OH peaks in 4a-dimethylaminobicyclo[4.2.0]-octan-

3a-ol was discussed.

IT 41441-83-2

RL: PRP (Properties)

(conformation and hydrogen bonding in, ir and NMR in relation to)

RN 41441-83-2 CAPLUS

CN Bicyclo[4.2.0]octan-3-ol, 4-(dimethylamino)-,

 $(1\alpha, 3\alpha, 4\beta, 6\beta)$ – (9CI) (CA INDEX NAME)

Relative stereochemistry.

L23 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:

1969:512248 CAPLUS

DOCUMENT NUMBER:

71:112248

TITLE:

Conformation and reactivity of trans-fused bicyclo [4.n.0] derivatives. VII. Elimination reactions of

trans-bicyclo [4.2.0] octane

AUTHOR(S):

Largeau, Claude; Casadevall, Andre; Casadevall,

Eliette

CORPORATE SOURCE:

Fac. Sci., Montpellier, Fr.

SOURCE:

Bulletin de la Societe Chimique de France (1969), (8),

2734-41

CODEN: BSCFAS; ISSN: 0037-8968

DOCUMENT TYPE:

Journal

LANGUAGE:

French

OTHER SOURCE(S):

CASREACT 71:112248

GI For diagram(s), see printed CA Issue.

AB trans-Bicyclo[4.2.0]octan-3-ols I are dehydrated (KHSO4) to give trans-bicyclo[4.2.0]oct-3-ene (II); the I and ZnCl2 give II-III mixts., where II is the major product. I xanthates are pyrolyzed to give II. I tosylates are treated with NaOMe-MeOH and tert-BuOK-tert-BuOH to give mixts. of II and the alkyl ethers of the I; the 3(a)-toxylate of I and

tert-BuOK-tert-BuOH give >99% II.

IT 25137-18-2P 25253-73-0P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of)

RN 25137-18-2 CAPLUS

CN Bicyclo[4.2.0]octan-3-ol, 4-(dimethylamino)- (8CI) (CA INDEX NAME)

RN 25253-73-0 CAPLUS

CN Bicyclo[4.2.0]octan-3-ol, 4-(dimethylamino)-, monopicrate (8CI) (CA INDEX NAME)

CM 1

CRN 25137-18-2 CMF C10 H19 N O

CM 2

CRN 88-89-1 CMF C6 H3 N3 O7

FILE 'CAOLD' ENTERED AT 14:36:34 ON 09 MAR 2005

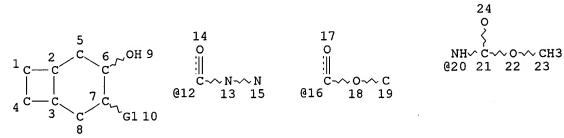
L24 0 S L22

FILE 'USPATFULL' ENTERED AT 14:36:45 ON 09 MAR 2005

L25 0 S L22

FILE 'MEDLINE, BIOSIS, EMBASE' ENTERED AT 14:36:53 ON 09 MAR 2005 L26 0 S L22

(FILE 'MARPAT' ENTERED AT 14:37:34 ON 09 MAR 2005) L27 STR



VAR G1=N/12/16/20 NODE ATTRIBUTES: DEFAULT MLEVEL IS ATOM DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RSPEC I

NUMBER OF NODES IS 23

STEREO ATTRIBUTES: NONE

ATTRIBUTES SPECIFIED AT SEARCH-TIME:

ECLEVEL IS LIM ON ALL NODES

ALL RING(S) ARE ISOLATED

L29 1 SEA FILE=MARPAT SSS FUL L27 (MODIFIED ATTRIBUTES)

100.0% PROCESSED 2037 ITERATIONS

1 ANSWERS

SEARCH TIME: 00.00.02

L29 ANSWER 1 OF 1 MARPAT COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:

136:369713 MARPAT

TITLE:

Preparation of 2-cyclohexylmethyl-, cyclohexylamino-, and cyclohexylaminomethylimidazopyridine as NMDA/NR2B

antagonists

INVENTOR(S):

Thompson, Wayne I.; Claremon, David A.; Munson, Peter

M.; Mccauley, John A.

PATENT ASSIGNEE(S):

Merck & Co., Inc., USA

SOURCE:

U.S. Pat. Appl. Publ., 44 pp., Cont.-in-part of U.S.

Ser. No. 6,291,499.

CODEN: USXXCO

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT: 3

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2002055519	A1	20020509	US 2001-861861	20010521
US 6495561	B2	20021217	•-	
US 6291499	B1	20010918	US 2000-696612	20001025
PRIORITY APPLN. INFO.	:		us 1999-162714P us 2000-696612	19991029 20001025

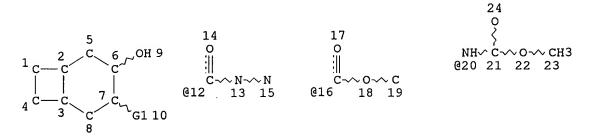
GI

$$\begin{array}{c|c}
 & X & A^2 \\
 & & L^2 \\
 & & R^2
\end{array}$$

AB 4-Substituted cyclohexanes substituted in the 1-position with imidazopyridine either directly or through a C1-4 alkyl, C1-4 alkenyl, C1-4 alkynyl, C1-4 alkoxy, amino, amino-C1-4 alkyl, hydroxy-C1-4 alkyl, carbonyl, cyclo-C3-6 alkyl or aminocarbonyl chain represented by general formula [I; R1 = 2-imidazopyridinyl optionally substituted with F, NH2, or HO; R2 = Ph, optionally substituted with one to five substituents, each substituent independently being C1, F, Br, C1-4 alkyl, CF3, HO, or CO2H; L1, L2 = independently C1-4 alkyl, C1-4 alkyl, C1-4 alkyl, C1-4 alkoxy, NH2, amino-C1-4 alkyl, hydroxy-C1-4 alkyl, carbonyl, C3-6 cycloalkyl, or aminocarbonyl; A1, A2, A3 are each hydrogen or (i) A1 and A2 form a two carbon bridge or (ii) A1 and A3 form a two carbon bridge; and optionally

substituted with X, wherein X is HO, NH2, C1-4 alkyl, di(C1-4alkyl)amino, C1-4 alkyl, ester, carbamate, carbonate, or ether] or pharmaceutically acceptable salt thereof are prepared These compds. are effective as N-methyl-D-aspartate (NMDA)/NR2B-subtype receptor antagonists and useful for relieving pain and for the treatment of migraine, depression, anxiety, schizophrenia, Parkinson's disease, or stroke. Thus, Wittig reaction of 4-benzylcyclohexane with 2-benzimidazolylmethyltriphenylphosphonium chloride in the presence of NaH in DMSO gave 2-(4-benzylcyclohexylidenemethyl)-1H-benzimidazole which was hydrogenated over 5% Pt/C in ethanol to give 2-(4-benzylcyclohexylmethyl)-1H-benzimidazole. In a FLIPR (fluorometric imaging plate reader) assay, selected compds. I inhibited NR1A/2B NMDA receptor-mediated Ca2+ influx in NR1A/2B NMDA receptor-transfected L(tk) cells with IC50 of <50 µM.

(FILE 'CASREACT' ENTERED AT 14:38:41 ON 09 MAR 2005)



VAR G1=N/12/16/20 NODE ATTRIBUTES: DEFAULT MLEVEL IS ATOM DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RSPEC I

L21

NUMBER OF NODES IS 23

STEREO ATTRIBUTES: NONE

L31 1 SEA FILE=CASREACT SSS FUL L21 (1 REACTIONS)

100.0% DONE 4203 VERIFIED 1 HIT RXNS 1 DOCS

SEARCH TIME: 00.00.01

L31 ANSWER 1 OF 1 CASREACT COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 71:112248 CASREACT

TITLE: Conformation and reactivity of trans-fused bicyclo

[4.n.0] derivatives. VII. Elimination reactions of

trans-bicyclo [4.2.0] octane

AUTHOR(S): Largeau, Claude; Casadevall, Andre; Casadevall,

Eliette

CORPORATE SOURCE: Fac. Sci., Montpellier, Fr.

SOURCE: Bulletin de la Societe Chimique de France (1969), (8),

2734-41

CODEN: BSCFAS; ISSN: 0037-8968

DOCUMENT TYPE: Journal LANGUAGE: French

GI For diagram(s), see printed CA Issue.

Trans-Bicyclo[4.2.0]octan-3-ols I are dehydrated (KHSO4) to give trans-bicyclo[4.2.0]oct-3-ene (II); the I and ZnCl2 give II-III mixts., where II is the major product. I xanthates are pyrolyzed to give II. I tosylates are treated with NaOMe-MeOH and tert-BuOK-tert-BuOH to give mixts. of II and the alkyl ethers of the I; the 3(a)-toxylate of I and tert-BuOK-tert-BuOH give >99% II.

RX(1) OF 1 A + B ===> C

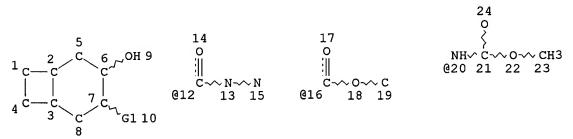
RX(1) RCT A 286-59-9, B 124-40-3

PRO C 25137-18-2

SOL 7732-18-5 Water

NTE Classification: Epoxide cleavage; C-Amination; # Conditions: H2O 120 deg 15h; # Comments: trans reactant

(FILE 'DJSMDS, CHEMINFORMRX' ENTERED AT 14:39:40 ON 09 MAR 2005) L21 STR



VAR G1=N/12/16/20 NODE ATTRIBUTES: DEFAULT MLEVEL IS ATOM DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RSPEC I

L27

NUMBER OF NODES IS 23

STEREO ATTRIBUTES: NONE L32 0 SEA L21

FILE 'MARPATPREV' ENTERED AT 14:44:55 ON 09 MAR 2005 STR

10/656617

VAR G1=N/12/16/20 NODE ATTRIBUTES: DEFAULT MLEVEL IS ATOM DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES: RSPEC I NUMBER OF NODES IS 23

STEREO ATTRIBUTES: NONE

ATTRIBUTES SPECIFIED AT SEARCH-TIME: ECLEVEL IS LIM ON ALL NODES ALL RING(S) ARE ISOLATED

O SEA FILE=MARPATPREV SSS FUL L27 (MODIFIED ATTRIBUTES) L33

100.0% PROCESSED 4 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

FILE 'HOME' ENTERED AT 14:45:16 ON 09 MAR 2005